Advanced Neutronics Simulation Development and Directions

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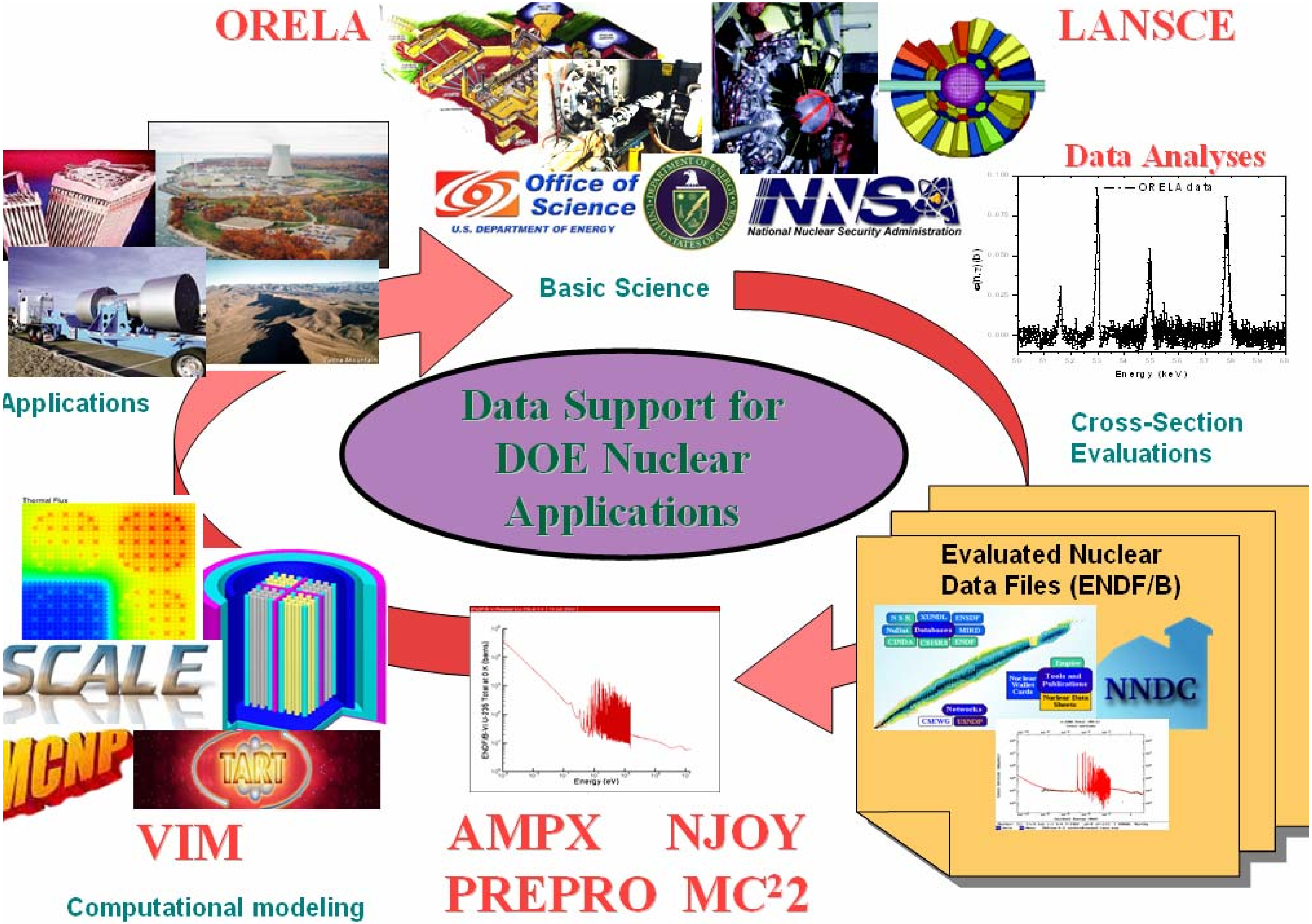
Topics

- **Nuclear Data**
- **Energy Treatment**
- **S/U Methods**
- **Optimization**
- **Nuclear Technology End Station Concept**



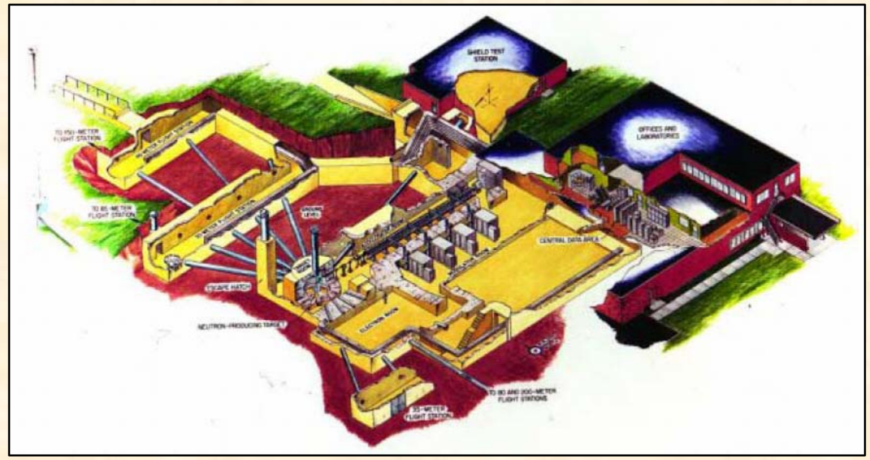
ORELA
LANSCE
Office of Science
U.S. DEPARTMENT OF ENERGY
NNSA
National Nuclear Security Administration
Data Analyses
ORELA data
Energy (keV)
Basic Science
Applications
Data Support for DOE Nuclear Applications
Cross-Section Evaluations
Evaluated Nuclear Data Files (ENDF/B)
NNDC
Energy (eV)
SCALE
MCNP
TART
VIM
AMPX
NJOY
PREPRO
MC²2
Computational modeling

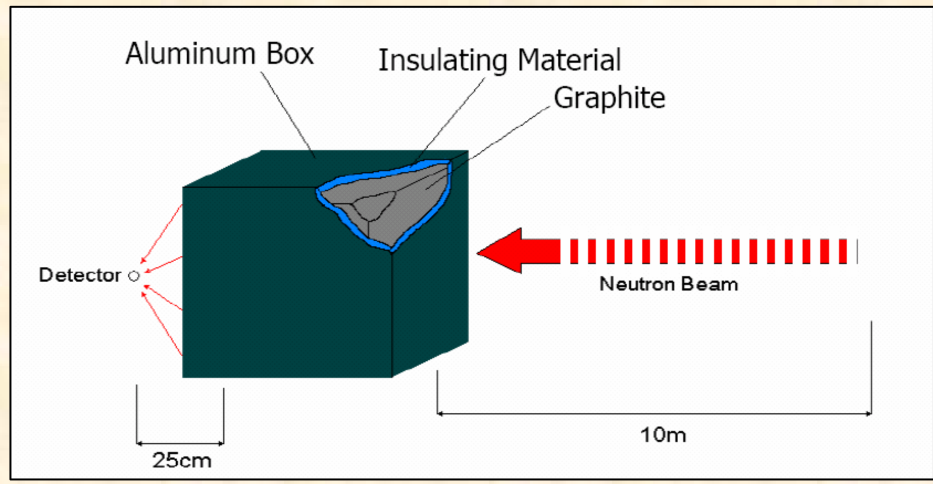
Development and Validation of Temperature Dependent Thermal Neutron Scattering Laws (NERI Project 01-140)

- **Collaborative Project with NCSU (Ayman Hawari) and Institute Balseiro, Argentina**
- **Update models and models' parameters by introducing new developments in thermalization theory and condensed matter physics**
  - **Use atomistic simulations to compute phonon distribution.**
  - **Use photon distribution in GASKET/LEAPR to compute updated scattering kernels (C, Be, BeO, ZrH, ThH, $(CH_2)_n$, H_2O**
- **Apply updated thermal scattering libraries to benchmark models to determine improvement.**
- **In the case of graphite, perform a benchmark experiment by observing neutron slowing down as a function of temperatures equal to or greater than room temperature**
- **Understand the implications of the obtained results on the ability to accurately determine the operating and safety Characteristics of a given reactor design**

ORELA Graphite Experiment

- **An experiment is currently being setup at ORELA to provide data for validation of the scattering kernels.**
- **A graphite pile is being placed in a furnace with Pu fission chambers and Li detectors to measure integral reaction rate vs time.**
- **Pulsed slowing down technique**
  - **Graphite pile (70-cm cubed) is set up in a furnace10 m from neutron source.**
  - **Measure integral reactor rate in detector as a function of time.**

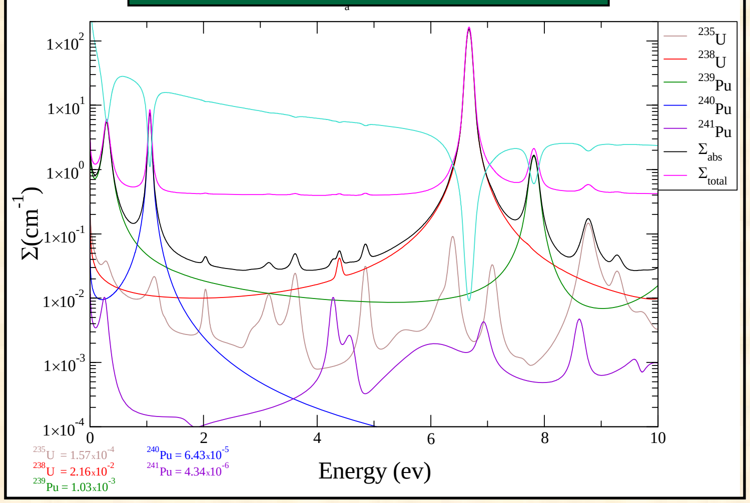




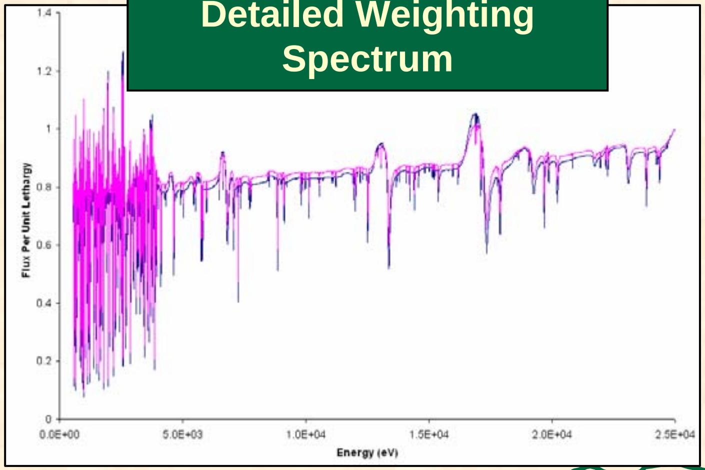
Improved Energy treatment in deterministic codes

- **1-D CENTRM Code introduced in SCALE 5.0**
  - **Continuous energy, point-wise library (~30,000 Energy Points)**
  - **Solve transport equation using Discrete Ordinates Method**
  - **Solve detailed slowing down problem to obtain multi-group cross sections for Monte Carlo/Lattice Physics Codes**

Resonance Overlap



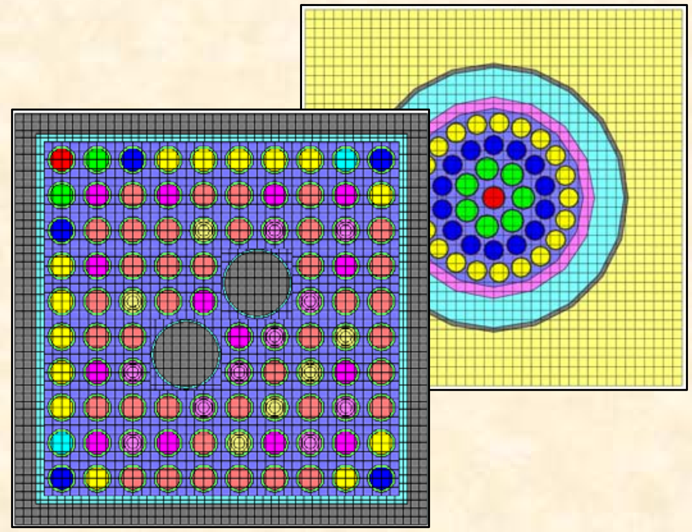
Detailed Weighting Spectrum

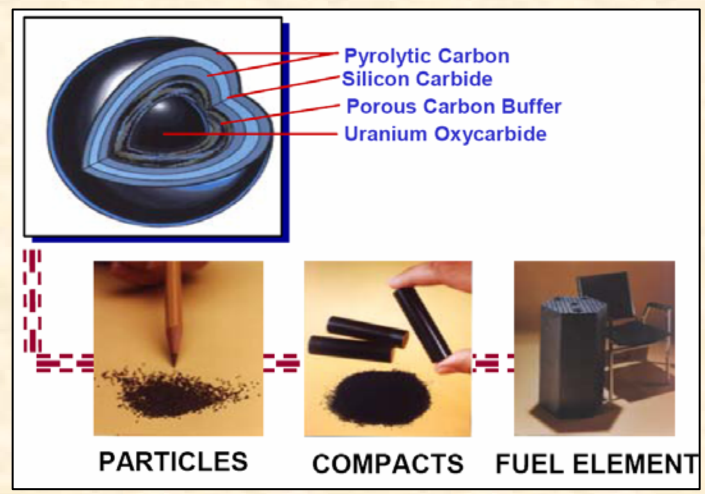


Detailed Energy Treatment – 2-D

- **1-D approximation cannot easily capture non-infinite lattices.**
- **GEMINEWTRN**
  - **Combine 2-D NEWT Extended Step Characteristics method with CENTRM Energy Detail**
  - **Idea for benchmarking more approximate methods**
- **Joint project with Purdue Univ.**

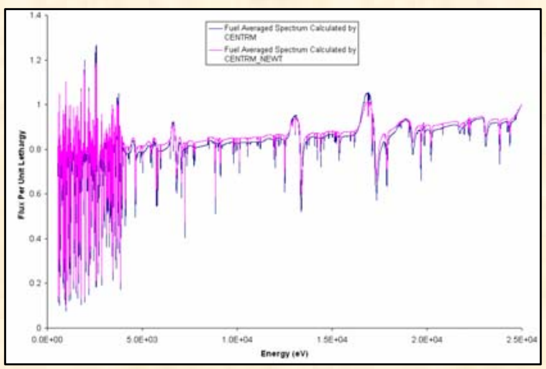
Heterogeneous Designs





TRITON Combines Rigorous Methods

- **CENTRM: 1-D continuous energy resonance processing**
- **ORIGEN-S: detailed isotopic compositions**
- **NEWT: 2-D flexible mesh geometry discrete ordinates transport**
- **Implemented in modular SCALE system**



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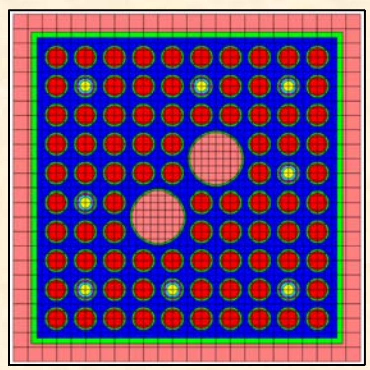

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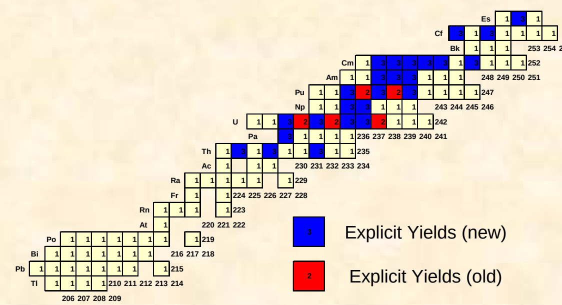


CENTRM (Energy Detail)

NEWT (Spatial/Angular Detail)

ORIGEN-S (Isotopic Detail, 1600 nuclides)

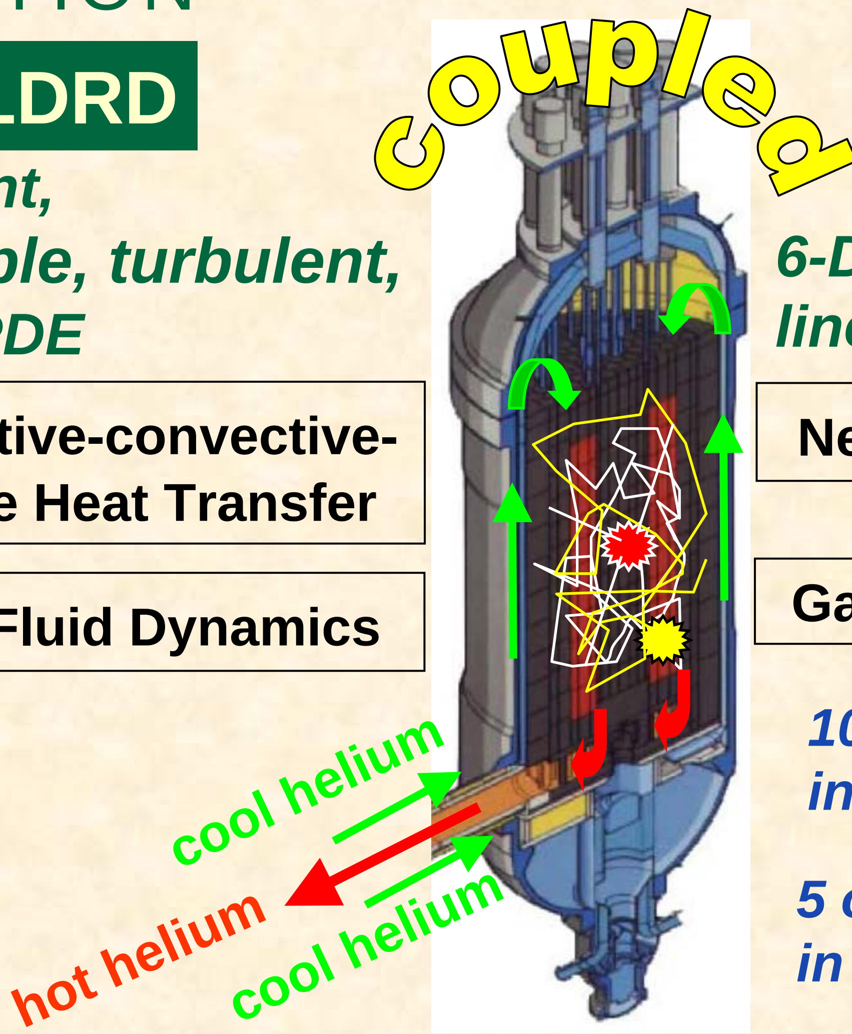
JOINT INL/ORNL LDRDs: FULLY-COUPLED NUCLEAR REACTOR SIMULATION

INL LDRD

3-D, transient, compressible, turbulent, non-linear PDE

Conductive-convective-radiative Heat Transfer

Fluid Dynamics



ORNL LDRD

6-D, transient linear integral-PDE

Neutron Transport

Gamma Transport

10 orders of magnitude in energy

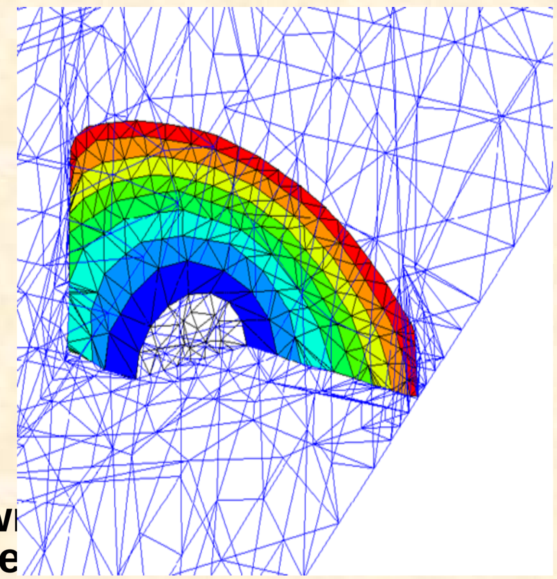
5 orders of magnitude in space

The ORNL LDRD: A HIGH-FIDELITY SIMULATION PACKAGE

- **Develop a high-fidelity radiation transport solver**
  - **Specifically designed for tera-scale computing**
  - **High-fidelity in both space and energy (based on centrm approach)**
- **Create the computer science infrastructure**
  - **For code efficiency & interoperability in terascale machines**
  - **Leverage existing software:**
    - **DOE's SciDAC software**
    - **ORNL's SCALE nuclear analysis code system**
  - **Teaming with ORNL computer science expertise**
- **Demonstrate the capability**
  - **Develop two visual demonstrations of the software**
    - **Independent radiation transport simulation**
    - **Coupled-physics simulation of a transient**

All built on a comprehensive COMPUTER SCIENCE INFRASTRUCTURE

- **Develop the setup geometry and meshing tools**
  - **Efficient parametric geometric modeling and processing tools**
  - **Advanced terascale grid generation and improvement techniques**
  - **Adaptive parallel hybrid mesh generation**
    - **Flexible mix of structured and unstructured mesh**
    - **AMR within the unified computational basis**
- **Leverage existing SciDAC technology**
  - **Common component architecture**
    - **Extensibility of each physics module**
    - **Interoperability of modules across platforms**
  - **Meshing tools and techniques from TSTT**
- **Domain decomposition and mesh ordering**
  - **Optimized ordering to take advantage of the *a priori* know computational wave fronts in the radiation transport solve**



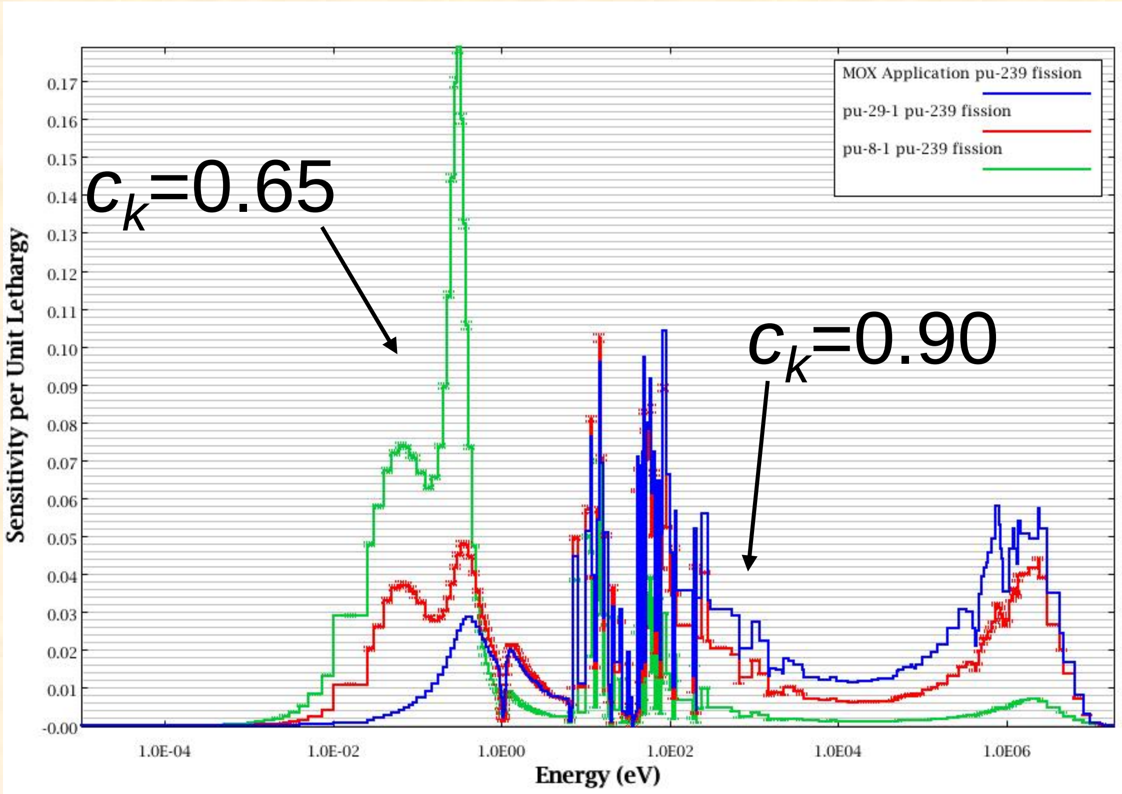
Validation, Experiments, and S/U

- **Good experiment data for code validation is hard to find for advanced reactor systems, a couple of key activities:**
  - **International Criticality Safety Benchmark Evaluation Project**
  - **International Reactor Physics Benchmark Experiments**
- **S/U tools can be used to determine:**
  - **What is important, which cross sections to measure**
  - **Fundamental assessment of uncertainties from basic data to support margins**
  - **Determine the applicability of experiments**
  - **Can be used to perform cross section adjustments to improve accuracy**

Example: Applicability of Experiments

- **Sensitivity data computed for experiments and applications for each reaction of each nuclide on energy-dependent basis.**
- **Integral indices assess degree of similarity between systems.**
- **Index range:**
  - **0.0: no similarity**
  - **1.0: identical**

^{239}Pu Fission Sensitivity Profiles: Sensitivity of k_{eff} to cross-section data on an energy-dependent basis



Optimization for Design

- **Current example is fuel loading**
- **With multi-physics, multi-component can apply optimization methods for automated design**
  - **Eliminate current iteration performed between particular areas of expertise**
  - **Computing intensive: requires multiple calculations**
  - **Optimize on economics, reliability, proliferation resistance**
- **Some general-purpose tools already exist (e.g. DAKOTA)**

Nuclear Technology End station Concept

1. **Approach for National Leadership Computing Facility - Complete simulation tool set on a HPC**
2. **Concept for reactor design and analysis:**

RADIATION TRANSPORT	CONTINUUM MECHANICS
Neutron	Multi-phase CFD
Photon	Heat transfer
	Chemically reactive flow
	Fluid-structure dynamics

3. **Add components for broader NS&T community**

RADIATION TRANSPORT	CONTINUUM MECHANICS
Charged-Particle	Elasto-plastic dynamics
Spallation Physics	Impact dynamics
	Radiation damage in materials